Methanone, [5-chloro-2-(methylamino)phenyl]phenyl-

Other names: Benzophenone, 5-chloro-2-(methylamino)-
[5-Chloro-2-(methylamino)phenyl]phenylmethanone
5-Chloro-2-(methylamino)benzophenone
2-Methylamino-5-chlorobenzophenone
Benzophenone, 2-acetamido-5-chloro-
2-Methylamino-5-chlorbenzophenone
Diazepam benzophenone
Diazepam, acid hydrolyzed

Inchi: InChI=1S/C14H12ClNO/c1-16-13-8-7-11(15)9-12(13)14(17)10-5-3-2-4-6-10/h2-9,16H,1H

InchiKey: WPNMLCMTDCANOZ-UHFFFAOYSA-N

Formula: C14H12ClNO

SMILES: CNc1ccc(Cl)cc1C(=O)c1ccccc1

Mol. weight [g/mol]: 245.70

CAS: 1022-13-5

Physical Properties

Property code	Value	Unit	Source
gf	221.10	kJ/mol	Joback Method
hf	42.98	kJ/mol	Joback Method
hfus	30.22	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.613		Crippen Method
mcvol	184.390	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2115.00		NIST Webbook

rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
tb	724.51	K	Joback Method
tc	972.24	K	Joback Method
tf	457.93	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.13	J/mol×K	724.51	Joback Method
cpg	476.46	J/mol×K	765.80	Joback Method
cpg	488.65	J/mol×K	807.09	Joback Method
cpg	499.77	J/mol×K	848.38	Joback Method
cpg	509.90	J/mol×K	889.66	Joback Method
cpg	519.12	J/mol×K	930.95	Joback Method
cpg	527.47	J/mol×K	972.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1022135&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume